Incorporating Reduced Ion Kinetic Models in Hydrodynamics Codes

Kinetic Physics 2016 Workshop

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Ion mean-free-path models "easily" implemented in hydro codes

- Ion heat conduction (energy diffusion)
- Ion viscosity (momentum diffusion)
- Ion species diffusion/separation (mass diffusion)
- Knudsen layer effects on TN burn rate
- Multiple ion temperatures
- Stress tensor evolution
- Kinetics inspired Coulomb cross-sections
- Multi-fluid (multi-velocity) hydro

Can these "simple" models capture most of the important effects?
Or do we need Fokker-Planck, Boltzmann or particle methods?

Ion heat conduction has been available for decades

- Uses same diffusion solver as electron heat conduction
  - Sparse matrix solve yields stability/positivity for all time steps

- Braginskii provides formulas for single species ion heat conductivity
  - Flux limit so that $q < v\ n\ Ti$

- Simplest extension to multiple species (~N work)
  - Assume single ion temperature
  - Use some "average" Coulomb logarithm
  - Sum heat flow over each species: $A^{-1/2}/Z^4 = \langle A^{-1/2}/Z^2 \rangle / \langle Z^2 \rangle$
  - Use some "average" $\omega\tau$ to correct for magnetic field effects

Should really be $2A_{reduced}$ for each ion pair

- A better extension to multiple species (~N^2 work, not completed)
  - Form all pairwise Coulomb logs (Stanton & Murillo fits for all coupling strengths)
  - Form τ and $\omega\tau$ separately for each species
  - Correct each species conductivity for magnetic effects and sum over species

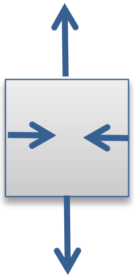
- Should include heat flow corrections due to species diffusion/separation

Magnetic corrections (~AZ^2) can vary widely between species.
Ion heat conduction can dominate electron heat conduction in strong fields.

Real ion viscosity has been available for decades

- Typically implemented explicitly in hydrodynamics codes
  - Stability time step $\Delta t = \Delta x^2 \rho/\eta$
  - Still need artificial viscosity to handle shocks when real viscosity is small
- Robinson & Bernstein, Annals of Physics **18**, 110 (1962) provides formulas for single species ion viscosity (tensor in magnetic field)
  - Flux limit so that stress tensor does not “suck”

$$\eta < \frac{3}{2} n_i T_i / \sqrt{\nabla \vec{v} : \nabla \vec{v}}$$



- Simplest extension to multiple species (~N work)
  - Use some average Ti, $\omega\tau$ and Coulomb log
  - Sum viscosity over each species: $A^{1/2}/Z^4 = \langle A^{1/2}/Z^2 \rangle / \langle Z^2 \rangle$
- A better extension to multiple species (~N^2 work, not completed)
  - Use pairwise Coulomb logs from ion conductivity (Stanton & Murillo)
  - Correct each species viscosity for magnetic effects and sum over species

Ion species diffusion/separation needs more work

- grad(Pe) & grad(Pi) have been there for decades
- grad(Te) & grad(Ti) were recently added – Thanks to Grisha Kagan for grad(Ti)
- So far the model is only correct for N=2 species
  - Written for any N
  - Reduces to the correct N=2 case wherever any two species dominate
  - May be nearly correct for some N>2 cases
  - Uses a "fixup" to assure zero total mass flux in Lagrange frame (needed for N>2)
  - Involves N^2 work to form grad(Ti) coefficients
  - Involves N^2 work to form binary diffusion coefficients for all ion pairs
  - Does not include any magnetic field effects
  - Uses split 1D sweeps to implement in multiple dimensions
- Possible future improvements
  - Upgrade binary diffusion coefficients from Paquette, et al. to Stanton & Murillo
  - Handle the N>2 cases correctly
  - Include consistent species diffusion effects on heat flow
  - Include magnetic fields effects

Simple model for species mass flux does not involve an NxN matrix because I have not figured out how to do that stably

$$\vec{F_s} = \sum_j n_s n_j R_{sj}\left(\vec{w_j} - \vec{w_s}\right) \approx -Q_s n_s m_s \vec{w_s} = -\,Q_s \vec{i_s}$$

$$= \nabla p_s - f_s^m \nabla p_i + (f_s^Z - f_s^m)\nabla p_e - \beta_{\parallel}^{uT}\left(f_s^{Z^2} - f_s^Z\right)\nabla T_e + \sum_j \rho f_s^m f_j^m \kappa_{sj}\left(\frac{f_s^m}{f_s^m + f_j^m}\right)\nabla T_i$$

Upwind implicit terms guarantee positivity for all time step

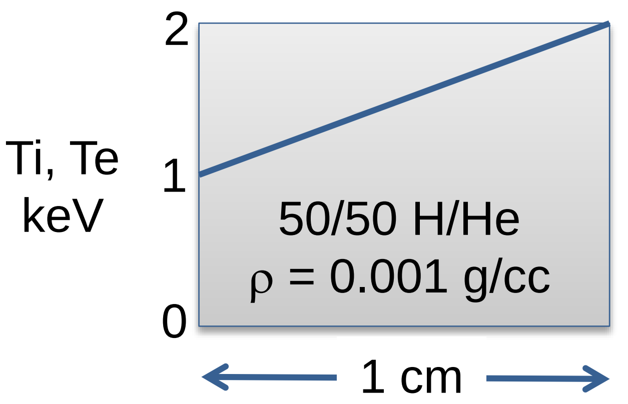
$$f_s^\alpha = \frac{n_s \alpha_s}{\sum_j n_j \alpha_j} \qquad \kappa_{sj}(c) = -\kappa_{js}(1-c) \qquad Q_s = \frac{\rho}{m_s}\frac{\sum_{j\neq s} n_j R_{sj}}{\sum_{j\neq s} n_j\, m_j}$$

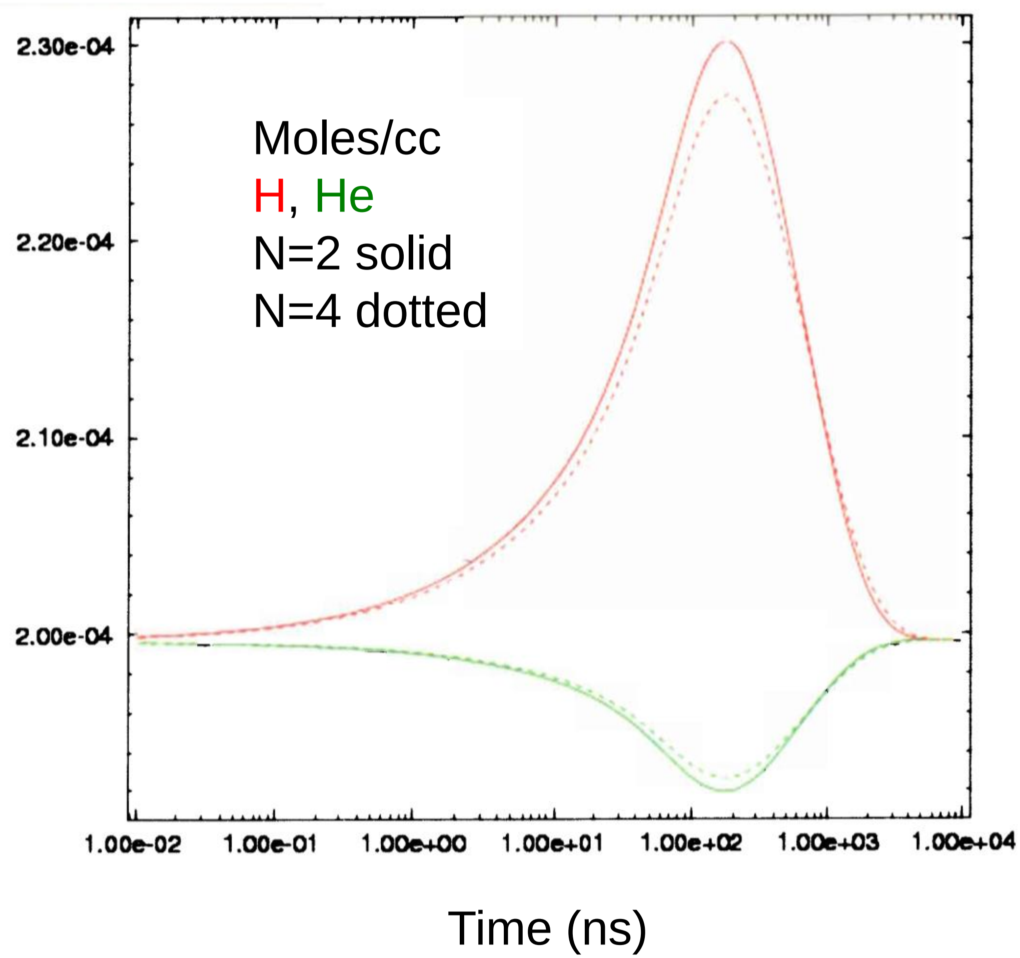
Correct for N=2

For several reasons the total mass flux is not zero, so do 2nd pass fixup

$$\overrightarrow{\Delta i_s} = -f_s^m \sum_j \vec{i_j}$$

Use colored H & He to test diffusion/separation for N=4 species





- No hydro or radiation
- No electron-ion coupling
- Include electron & ion heat conduction
- Record ion densities as a function of time at left end

We get agreement to 10% between N=2 and N=4 solutions

Some energy equation effects of ion species diffusion/separation are obvious from multi-fluid hydrodynamics

- In the Lagrange (zero mass flux) frame there are ion & electron number fluxes, $\vec{f}_{i,e}$=$n_{i,e}\vec{w}_{i,e}$, leading to energy fluxes of $3/2T_{i,e}\vec{f}_{i,e}$
- The single fluid hydrodynamics did ion & electron $P\nabla \cdot \vec{v}$ work using the mass weighted velocity, so they need to be corrected by $P_{i,e}\nabla \cdot \vec{w}_{i,e}$
- Frictional drag between ion species heats the ions $\left(\sum_s \vec{F_s} \cdot \vec{w_s} < 0\right)$
- After some math these conserve energy & result in ion & electron energy sources of

$$\dot{S}_i = -\nabla \cdot \sum_s A_{is}\vec{w_s}T_i + \Delta_{ei}$$

$$A_{is} = \frac{5}{2}n_s + \sum_j \rho f_s^m f_j^m \kappa_{sj}\left(\frac{f_s^m}{f_s^m + f_j^m}\right)$$

$$\Delta_{ei} = -\vec{w_e} \cdot \nabla p_e + \beta_{\parallel}^{uT} \sum_s \left(f_s^{Z^2} - f_s^Z\right)\vec{w_s} \cdot \nabla T_e$$

$$\dot{S}_e = -\nabla \cdot \sum_s A_{es}\vec{w_s}T_e - \Delta_{ei}$$

$$A_{es} = \frac{5}{2}n_s Z_s - \beta_{\parallel}^{uT}\left(f_s^{Z^2} - f_s^Z\right)$$

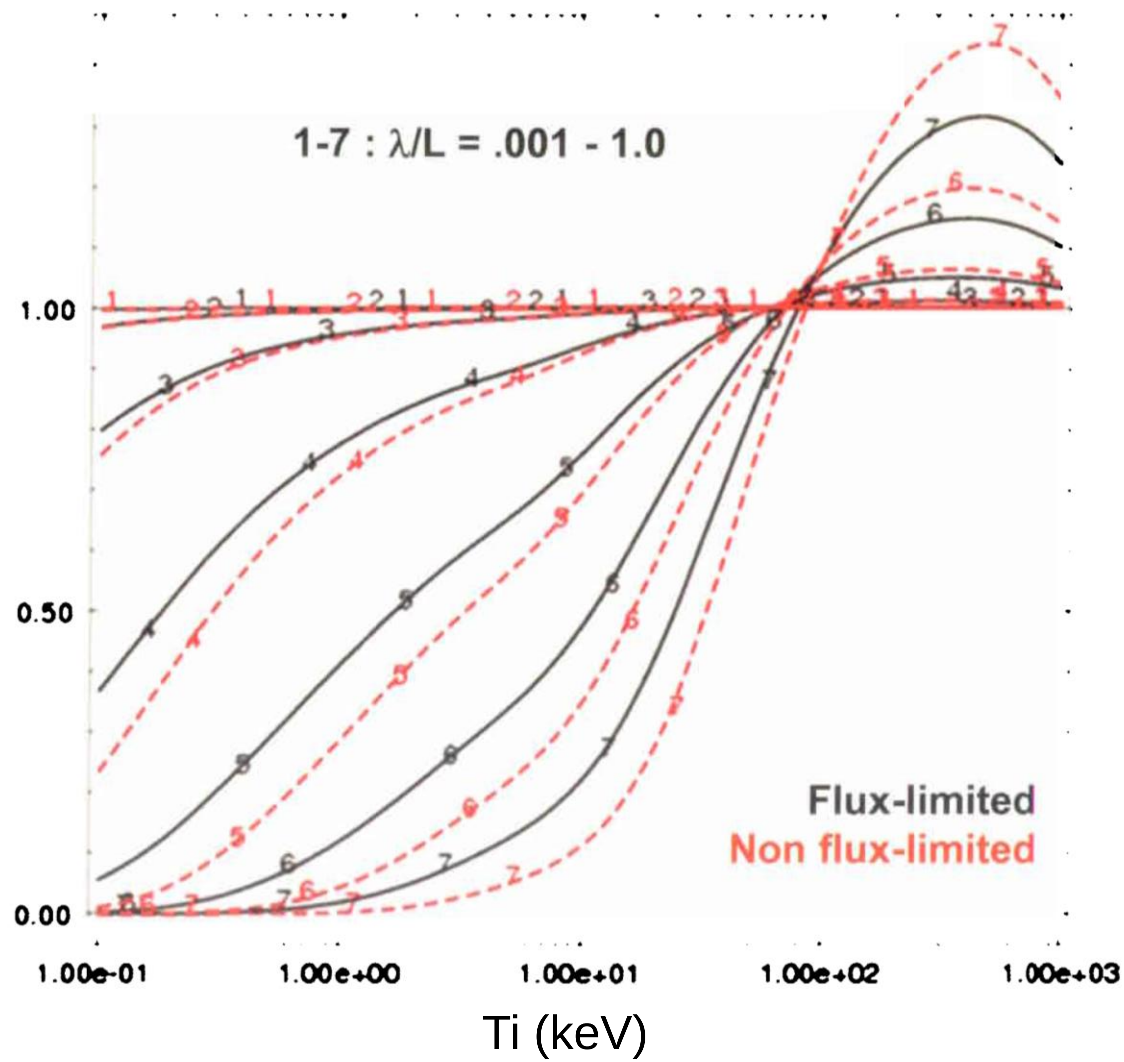
$$\vec{w_e} = \sum_s n_s Z_s \vec{w_s}/n_e$$

We get electron-ion heat exchange as well as heat flow.

Knudsen layer DT burn rate “reduction” factor

- Similar to model of Molvig, et al., PRL **109**, 095001 (2012)
- Sensitive to λ/L = thermal ion mfp / scale length
- With ion species diffusion on there is no “distance to wall” so I prefer

$$\frac{1}{L^2} = -\frac{1}{T_i}\nabla^2 T_i$$



Multiple ion temperatures may allow us to model more non-equilibrium effects

- Can we maintain two ion Maxwellians at different temperatures?
  - Yes, for $Z_H/Z_L = A_H/A_L = 100$ & $N_L/N_H = 3162$
  - NRL Plasma Formulary gives $\nu_\epsilon^{L/L}/\nu_\epsilon^{L/H} = \nu_\epsilon^{H/H}/\nu_\epsilon^{H/L} = 31.62$
  - So $T_L \neq T_H$ is possible, but not as ubiquitous as $Te \neq Ti$

- How do we drive an ion temperature separation?
  - Electron-ion coupling will only produce T_H-T_L ~ 1/43 (Te-Ti)
  - Alpha stopping to ions goes like Z^2/A, so maybe
  - Adiabatic compression & expansion preserves T_L/T_H, so nothing there
  - Shock heating is proportional to A, so this may be the big one
  - Ion heat conduction can yield $(T_H-T_L)/T_L = A_H/A_L\,(\lambda_L/L)^2$, so this could matter

- Models that need to be generalized for multiple Ti (WIP by Dan Klem)
  - EOS, adiabatic & shock heating
  - TN burn rates & burn product deposition
  - Electron-ion & ion-ion coupling
  - Ion heat conduction, viscosity & species diffusion/separation
  - Doppler line broadening, some LPI stuff, …

Simplest multi ion heat conduction gives no heat across species discontinuities !!!

Some hydrodynamic extensions may also be useful

- Stress tensor evolution includes the inertia of the ion anisotropy
  - Provides non-hydrodynamic effects even within a single fluid
  - I believe this can be done explicitly with $\Delta t \propto \Delta x$ instead of viscosity's $\Delta t \propto \Delta x^2$
  - If $\Delta t \sim \Delta t_{Courant}/3^{½}$ then this might be worth doing even if it is no better physically than viscosity

- Kinetics inspired Coulomb cross-sections includes bulk velocity in collision velocity
  - Thanks to Peter Amendt for the idea
  - Important when $\lambda|\nabla\vec{v}| > 1$
  - Generally decreases Coulomb cross-section making itself more important
  - Requires a non-local operator to get velocity jump across one mfp
  - Current (very crude upper limit) uses v instead of Δv & is not Galilean invariant

- Multi-fluid (multi-velocity) hydro
  - Naturally includes the above effects
  - But only for collisional processes between different fluids

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